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Modified Verlet Method Involving Second-Order Mid-Point Rule Applied to Balls Falling in One-Dimensional Potentials

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Abstract. A modified Verlet method which involves a kind of mid-point rule is constructed and applied to the one-dimensional motion of elastic balls of finite size, falling under constant gravity in space and then under the chemical potential in the interface region of phase separation within a two-liquid film. When applied to the simulation of two balls falling under constant gravity in space, the new method is found to be computationally superior to the usual Verlet method and to Runge–Kutta methods, as it allows a larger time step for comparable accuracy. The main purpose of this paper is to develop an efficient numerical method to simulate balls in the interface region of phase separation within the two-liquid film, where the ball motion is coupled with two-phase flow. The two-phase flow in the film is described via shallow water equations, using an invariant finite difference scheme that accurately resolves the interface region. A larger time step in computing the ball motion, more comparable with the time step in computing the two-phase flow, is a significant advantage. The computational efficiency of the new method in the coupled problem is demonstrated for the case of four elastic balls in the two-liquid film.

AMS subject classifications: 65L12, 65M06, 65P10

Key words: Verlet method, falling balls, first return map, phase separation, shallow water equations.

1. Introduction

The main purpose of this paper is to develop an efficient numerical method to simulate the motion of elastic balls of finite size in immiscible two-liquid films. The phase separates in immiscible films, and the balls are expected to align near the phase separation interface in a kind of self-organisation process related to problems of nanotechnology [8, 18]. Since film phenomena are quite complex, the simulation in this paper is restricted to one

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dimension – i.e. the balls (that may collide) fall in a straight line to the bottom of the phase separation potential in the two-phase flow.

Falling ball problems are not easy to analyse. However, balls falling in space under constant gravity have been studied with reference to ergodic theory [4]. In the case of point masses moving in one dimension above a fixed floor, when the upper point masses are lighter than the lower ones it has been proven mathematically that the system has some non-vanishing Lyapunov exponents almost everywhere, and becomes chaotic [16,17]. For two point masses, there is typical Kolmogorov–Arnold–Moser behaviour when the upper mass is heavier than the lower one, where quasi-periodic and chaotic trajectories coexist in the phase space [15]. Related numerical integration must be performed with high accuracy, and lengthy simulations of falling balls have been undertaken using the symplectic Verlet method.

The main difficulty encountered in previous simulations of the motion of elastic balls of finite size in immiscible two-liquid films was the significantly smaller time step required in the Verlet method than the time step permitted for the flow computation by the CFL (Courant-Friedrichs-Lewy) condition, for a given accuracy. This led the author to construct the modified Verlet method involving the second-order mid-point rule adopted in this paper – i.e. to allow larger time steps for the simulation of the ball motion, more compatible with the time steps allowed in the invariant finite difference scheme used to solve the two-phase shallow-water equations invoked [14].

2. Two Balls Falling Under Constant Gravity and the Modified Verlet Method Involving the Second-Order Mid-Point Rule

In this Section, the modified Verlet method involving the second-order mid-point rule is constructed and applied to the case of two elastic balls of finite size falling vertically under constant gravity above a fixed rigid horizontal floor. This new method is first used in two simpler test problems – viz. the harmonic oscillator and the case of a single bouncing ball. When applied to the two balls falling in space, the new method is then shown to be more efficient than either the usual Verlet or various Runge-Kutta methods.

2.1. Mathematical model

The motion of two balls falling in one dimension under constant gravity above the fixed floor is governed by the system of equations

$$\frac{dz_i}{dt} = v_i \,, \tag{2.1}$$

$$\frac{dv_i}{dt} = f_i\left(z_1, z_2\right) \,, \quad i = 1, 2. \tag{2.2}$$

Here z denotes the vertical position of a ball above the horizontal floor, v the corresponding vertical velocity of the ball, t the time, f represents the acceleration, and the subscripts 1